inertia of the CO molecule about its CM is then (see Example 8–10)

$$I = m_1 r_1^2 + m_2 r_2^2$$
$$= \left[(12\,\text{u})(0.57r)^2 + (16\,\text{u})(0.43r)^2\right]\left[1.66 \times 10^{-27}\,\text{kg/u}\right]$$
$$= \left(1.14 \times 10^{-26}\,\text{kg}\right)r^2.$$

We solve for r and use the result of part (a) for I:

$$r = \sqrt{\frac{1.46 \times 10^{-46}\,\text{kg}\cdot\text{m}^2}{1.14 \times 10^{-26}\,\text{kg}}} = 1.13 \times 10^{-10}\,\text{m} = 0.113\,\text{nm}.$$

EXERCISE A What are the wavelengths of the next three rotational transitions for CO?

* Vibrational Energy Levels in Molecules

The potential energy of the two atoms in a typical diatomic molecule has the shape shown in Fig. 29–8 or 29–9, and Fig. 29–17 again shows the PE for the H_2 molecule (solid curve). This PE curve, at least in the vicinity of the equilibrium separation r_0, closely resembles the potential energy of a harmonic oscillator, PE $= \frac{1}{2}kx^2$, which is shown superimposed in dashed lines. Thus, for small displacements from r_0, each atom experiences a restoring force approximately proportional to the displacement, and the molecule vibrates as a simple harmonic oscillator (SHO)—see Chapter 11. According to quantum mechanics, the possible energy levels are quantized according to

$$E_{\text{vib}} = \left(\nu + \tfrac{1}{2}\right)hf, \qquad \nu = 0, 1, 2, \cdots, \tag{29–3}$$

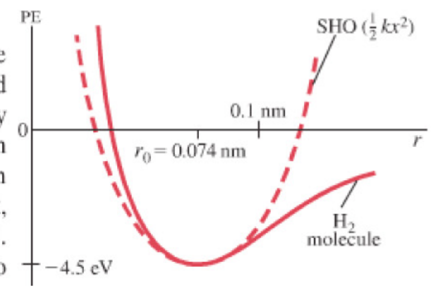


FIGURE 29–17 Potential energy for the H_2 molecule and for a simple harmonic oscillator (PE $= \frac{1}{2}kx^2$, with $|x| = |r - r_0|$).

where f is the classical frequency (see Chapter 11—f depends on the mass of the atoms and on the bond strength or "stiffness") and ν is an integer called the **vibrational quantum number**. The lowest energy state ($\nu = 0$) is not zero (as for rotation), but has $E = \frac{1}{2}hf$. This is called the **zero-point energy**. Higher states have energy $\frac{3}{2}hf$, $\frac{5}{2}hf$, and so on, as shown in Fig. 29–18. Transitions are subject to the *selection rule*:

Selection rule (vibrational energy)

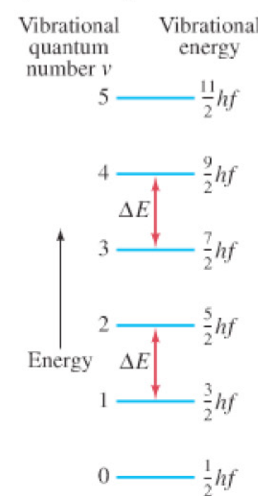
$$\Delta\nu = \pm 1,$$

so allowed transitions occur only between adjacent states, and all give off photons of energy

$$\Delta E_{\text{vib}} = hf. \tag{29–4}$$

This is very close to experimental values for small ν, but for higher energies, the PE curve (Fig. 29–17) begins to deviate from a perfect SHO curve, and this then affects the wavelengths and frequencies of the transitions. Typical transition energies are on the order of 10^{-1} eV, about 10 times larger than for rotational transitions, with wavelengths in the infrared region of the spectrum ($\approx 10^{-5}$ m).

FIGURE 29–18 Allowed vibrational energies for a diatomic molecule, where f is the fundamental frequency of vibration (see Chapter 11). The energy levels are equally spaced. Transitions are allowed only between adjacent levels ($\Delta\nu = \pm 1$).



EXAMPLE 29–3 Vibrational energy levels in hydrogen. Hydrogen molecule vibrations emit infrared radiation of wavelength around 2300 nm. (a) What is the separation in energy between adjacent vibrational levels? (b) What is the lowest vibrational energy state?

APPROACH The energy separation between adjacent vibrational levels is (Eq. 29–4) $\Delta E_{\text{vib}} = hf = hc/\lambda$. The lowest energy (Eq. 29–3) has $\nu = 0$.

SOLUTION

$$(a)\ \Delta E_{\text{vib}} = hf = \frac{hc}{\lambda} = \frac{\left(6.63 \times 10^{-34}\,\text{J}\cdot\text{s}\right)\left(3.00 \times 10^{8}\,\text{m/s}\right)}{\left(2300 \times 10^{-9}\,\text{m}\right)\left(1.60 \times 10^{-19}\,\text{J/eV}\right)} = 0.54\,\text{eV},$$

where the denominator includes the conversion factor from joules to eV.
(b) The lowest vibrational energy has $\nu = 0$ in Eq. 29–3:

$$E_{\text{vib}} = \left(\nu + \tfrac{1}{2}\right)hf = \tfrac{1}{2}hf = 0.27\,\text{eV}.$$

EXERCISE B What is the energy of the first vibrational state above the ground state in the hydrogen molecule?